

CIRCULATION COPY
SUBJECT TO RECALL
IN TWO WEEKS

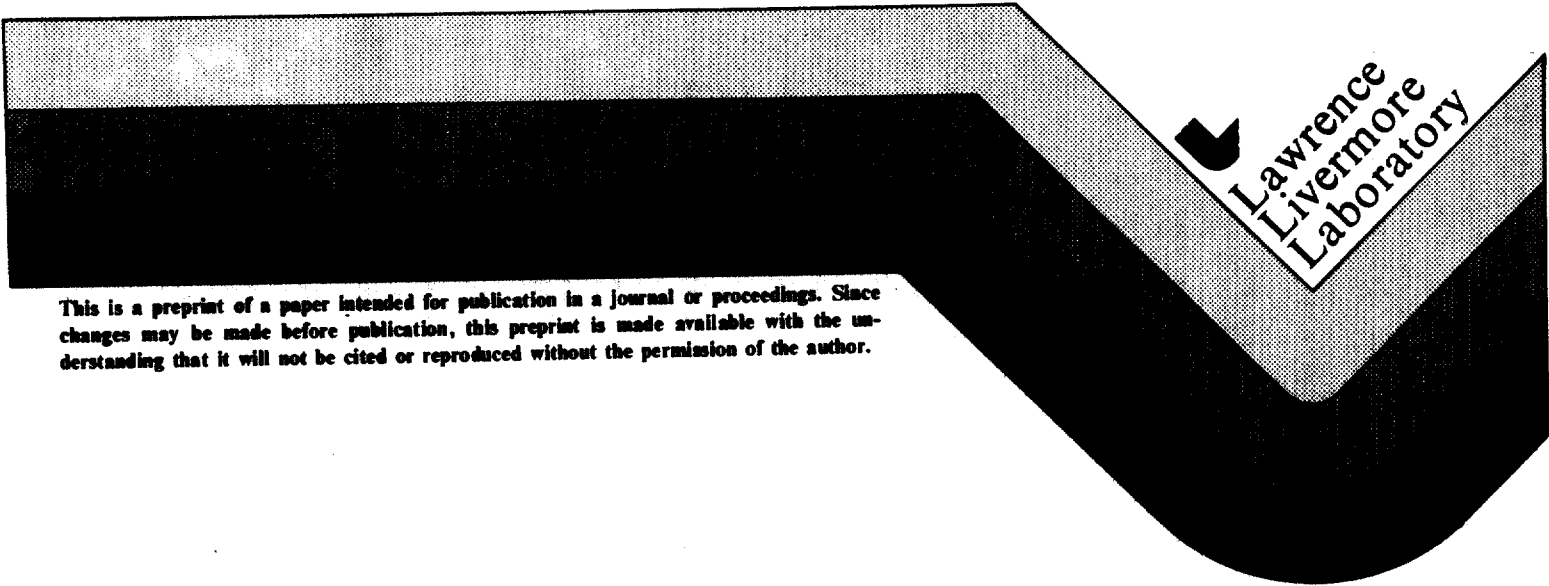
UCRL-82529
PREPRINT

APPLICATIONS OF MODERN CONTROL THEORY TO PROCESS CONTROL

Charles J. Herget
Jack W. Frazer

This paper was prepared for submission to IEEE Conference on
Decision and Control, at Fort Lauderdale, Florida on December 12-14, 1979.

August 29, 1979

The logo for Lawrence Livermore Laboratory is a large, stylized 'L' shape. The top horizontal bar of the 'L' is light gray, while the vertical stem and the bottom curve are black. The text 'Lawrence Livermore Laboratory' is written in a sans-serif font, oriented diagonally along the right side of the vertical stem.

Lawrence
Livermore
Laboratory

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

APPLICATIONS OF MODERN CONTROL THEORY TO PROCESS CONTROL*

Charles J. Herget and Jack W. Frazer†

Lawrence Livermore Laboratory
University of California
Livermore, CA 94550

Abstract

This paper contains a brief description of research on the control of an enzyme reactor at the Lawrence Livermore Laboratory. One of the objectives of the research is to develop improved design methods for use in the chemical industry in order to increase productivity and efficiency in laboratory, pilot plant, and production facilities. A laboratory bench scale apparatus with a problem environment similar to that found in a commercial pilot plant has been built, and an interdisciplinary team of engineers, chemists, and mathematicians has been organized. This paper describes the project and some of its goals.

Introduction

The application of modern control theory to control of chemical processes has been slow in spite of the potential benefits of successful implementation. Control algorithms which were previously attainable only on large scientific computers can now be implemented on inexpensive microcomputers that are on-line to the process and instrumentation monitoring the process. Most digital control algorithms have simply been replacements for old analog circuitry. Progress has been slow, in part, because of the complexity of chemical systems and the lack of communication between associated disciplines. Demonstration of successful applications of modern control theory on experimental systems is needed.

Typical complexities encountered in the control of chemical processes are the large number of process variables, strong interaction among variables, process delays, lack of good control models, need to incorporate control bounds in the design, and system disturbances and noise which are difficult to characterize. In order to provide a systematic procedure to approach these difficult problems, a laboratory bench scale apparatus with a problem environment similar to that found in a commercial pilot plant has been built, and an interdisciplinary team of engineers, chemists, and mathematicians has been organized at the Lawrence Livermore Laboratory. The goals are to be able to rapidly characterize complex chemical reactions, determine optimum operating conditions, and develop control algorithms to achieve these optimum conditions under adverse conditions.

*Work performed under the auspices of the Department of Energy by Lawrence Livermore Laboratory under contract W-7405-ENG-48.

†Author to whom all correspondence should be addressed.

System Description

Enzyme catalyzed reactions were selected for initial experimentation because they have a large number of variables with complex interactions. A functional block diagram of the computer controlled enzyme reactor is shown in Fig. 1. Input reagents are pumped into the experimental reactor via stepping motors whose pumping rates are controlled by a digital computer. Available inputs are enzyme, substrate, inhibitor, buffer, and diluent. A series of four delay loops and valves permit sixteen possible path lengths which determine the time for the reaction to occur. The absorption of the product is measured by a spectrophotometer located at the end of the delay lines. The output of the spectrophotometer is sampled, converted to digital form, and input to the digital computer. The concentration of the product is determined from the absorption. The measured absorption is fed back to the controller which determines the rate at which to pump the reagents, thus completing the feedback loop. In the initial experiments, enzyme has been the only variable used for control. Substrate concentration is held constant, and pH is held constant by pumping buffer at the appropriate rate. A block diagram which illustrates each of the functions just described is shown in Fig. 2.

In the experimental work done to date, the enzyme used is alkaline phosphatase, the substrate is p-nitrophenylphosphate, the buffer is 2-amino-2-methyl-1-propanol, the diluent is water, and no inhibitor is added. The product formed is p-nitrophenylate.

Modeling and Control

The initial effort has been concerned with the modeling and control of systems with large time delays. Single input control is being studied first with enzyme concentration being the control variable. Substrate concentration and pH are held constant. A dynamic model relating product concentration to enzyme concentration has been found using a nonlinear least squares parameter identification technique [1]. A linear second order model plus delay has been found to give a good representation of the actual system. The model was found using open loop tests by varying the rate of enzyme added. Since the pumping motors have limited pumping rates, the control system is nonlinear in the closed loop mode.

The method introduced by O. J. M. Smith [2] for designing linear systems with time delays has been extended to a more general class of multivariable, nonlinear, sampled data systems. As with the classical Smith predictor, the control design is based on the system model without time delay.

The time optimum control provides a nontrivial demonstration of the methods of modern control theory. A slightly modified version of Desoer and Wing's algorithm [3] for the control of saturating sampled data systems was implemented. The problem of interest is to move from one set point to another in minimum time. Because of the mismatch which will always exist between the model and the actual system, some form of corrective feedback is desirable after the completion of the time optimum sequence in order to maintain the new set point. A useful controller for maintaining the set point which is quite insensitive to modeling errors is the proportional plus integral plus derivative (PID) controller. The control strategy was to use a time optimum control sequence immediately after a step change in set point. At the time at which the time optimum control would want to switch to its final value, PID control was switched in.

A typical response is shown in Fig. 3. For comparison, the step response of the system under PID control only is also shown. It can be seen that the time optimum controller provides considerable improvement in achieving the new set point and that the time optimum control is very sensitive to modeling errors.

Future Studies

Multi-input systems in which both enzyme and substrate are available for control will be studied next. Models will be found by parameter identification methods, and various modern control strategies will be tested. Later, pH will be treated as one of the control variables. Experiments have shown that the system is highly nonlinear with respect to variations in pH. A primary concern in all of the research is to relate all models to the chemical reactions which are taking place. The characterization of the chemistry is a parallel effort [4] which will be incorporated into the control in future studies.

On-line identification of variations or upsets in the chemicals is a topic for future study. An adaptive controller which will adjust for upsets in the chemicals is another of the goals.

References

1. C. L. Pomernacki, *et al.*, "Characterization of the Flow Dynamics of an Enzyme Reaction System," accepted for publication in *Anal. Chim. Acta, Computer Techniques and Optimization*, 1979.
2. O. J. M. Smith, "A Controller to Overcome Dead Time," *Instrument Society of America Journal*, V. 6, 1959, pp. 28-33.
3. C. A. Desoer and J. Wing, "An Optimal Strategy for a Saturating Sampled Data System," *IRE Transactions on Automatic Control*, V. AC-6, 1961, pp. 5-15.
4. J. W. Frazer, *et al.*, "Characterizing Chemical Systems with On-Line Computers and Graphics," accepted for publication in *Anal. Chem.*, 1979.

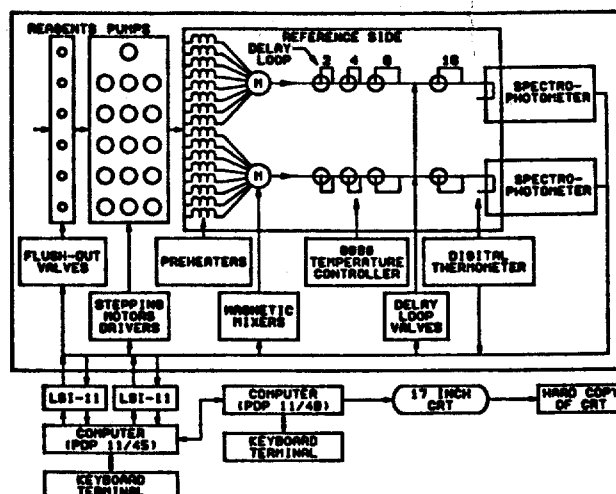


Fig. 1. Functional block diagram of the computerized apparatus showing the flow system and major components

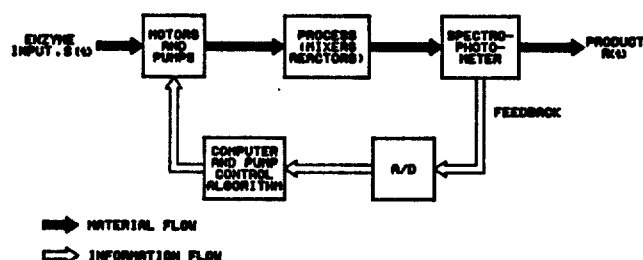


Fig. 2. Block diagram of the enzyme control system

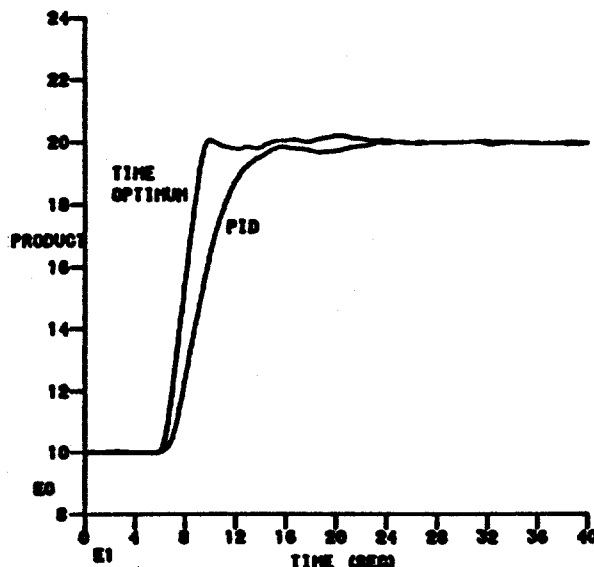


Fig. 3. Response of system with time optimum control followed by PID